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Connecting the Micro to the Mesoscale: Review and Specific Examples

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CONNECTING THE MICRO TO THE MESOSCALE: REVIEW AND SPECIFIC EXAMPLES

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1. Introduction

Historically, dislocation are thought of and treated as dual objects. The large lattice distortions inside the core region warrant an atomistic treatment, whereas the slightly distorted crystal outside of the core is well represented within a linear elastic framework. Continuum dislocation theory is powerful and elegant. Yet, it is unable to fully account for the structural differentiation of dislocation behavior, say, within the same crystallography class. The source of these structural variations is mostly in the dislocation core (see [1] for an excellent review).

In the past several years, the gap between the two approaches (atomistic and continuum-mesoscopic) for modeling dislocation behavior has started to close, owing to the overlap of the time and length scales accessible to them [2]. The current trend in dislocation modeling is to try to abstract the local rules of dislocation behavior, including their mobility and interactions, from the atomistic simulations and then incorporate these rules in a properly defined continuum approach, e.g. Dislocation Dynamics. The hope is that, by combining the two descriptions, a truly predictive computational framework can be obtained. For this emerging partnership to develop, some interesting issues need to be resolved concerning both physics and computations. It is from this angle that I will try to discuss several recent developments in atomistic simulations that may have serious implications for connecting atomistic and mesoscopic descriptions of dislocations. These are intended to support my speculations on what can and should be expected from atomistic calculations in

the near future, for further development of dislocation theory of crystal plasticity.

2. Single dislocation behavior

Some of the important issues concerning single dislocations are core structure and energetics and the atomic modes of dislocation mobility.

2.1. CORE PROPERITES

Static core properties were analyzed in the past using empirical interatomic potentials [3]. More recently, semi-empirical Tight Binding (TB) and Density Functional Theory (DFT) methods were used to analyze dislocation core in silicon and other semiconductors [4,5]. Silicon, in particular, turned out to be an exceptionally “friendly” material for dislocation modeling. This is mostly due to the relatively low plane-wave cut-off energies (for total energy DFT calculations) that can be used in combination with large (hundreds of atoms) supercells. Because dislocation cores in Si are so extremely narrow, these supercells are sufficient to comfortably accommodate one or two dislocations, without core overlap.

Current capabilities of the DFT methods in combination with the rapidly increasing CPU throughput are becoming sufficient for ever more challenging tasks, such as modeling dislocation cores in BCC transition metals from first principles. The latter is an important target in the context of low temperature/high strain rate yield behavior in these materials determined mostly by the mobility of screw dislocations. The screw mobility, in turn, depends critically on the subtle details of the core structure which is poorly described by the interatomic potentials. In general, core contribution to the line energy (as required for the mesoscopic modeling) can and should be accurately evaluated as a function of dislocation character, using interatomic potentials and TB models and, in a near future, first principles methods. Recent calculations suggest that variations of the line energy with the character angle are non-monotonic [6], showing cusp-like features similar to the dependence of the grain boundary energy on the misorientation angle: the cusps follow the low index line directions (for dislocations), similar to the low sigma mis-orientations (for grain boundaries). For comparison, the elastic part of the line energy depends monotonically on the dislocation character. These angular "core modulations” of the line energy are related to the depth of the Peierls valleys

along the low index line directions and should affect the ways in which dislocations move through the lattice.

2.2. DISLOCATION MOBILITY

The major obstacle for realistic modeling of dislocation motion is the gap between the time scales of a typical MD simulation and those of the dislocation motion. Only when dislocation mobility is high, as in FCC metals at high temperatures, and only using computationally inexpensive interatomic potentials, can MD simulations be up to the task. Even in such special cases, in addition to the issue of inaccurate potentials, the electron scattering component of the drag force is missing and should be added separately to the phonon drag as an external parameter. On the other hand, when dislocation mobility is low, as in semiconductors or bcc transition metals (screw dislocations at low temperatures), MD simulations become ineffective – dislocations do not move on the nanosecond time scale of a typical MD simulation run. In such situations, Transition State Theory (TST) is a more appropriate frame for the analysis of infrequent dislocation translations [5].

Activation pathways of the kink mechanisms of dislocation motion in silicon have been studied in considerable detail. One important observation was that kink mechanisms of dislocation motion can be multiple and complex [3,4]. A general methodology for *a priori* analysis of possible kink species in the dislocation core was recently suggested, based on the consideration of broken-symmetries in the dislocation core [7]. Since no three-dimensional kink calculations are required for such an analysis, it can be used to predict geometrical characteristics of the possible kinks using accurate *ab initio* calculations of core structures. For silicon, a complete catalog of kink mechanisms was obtained including kink formation and migration energies. Based on this data, a detailed kinetic Monte Carlo (kMC) model of the dissociated dislocation was developed, combining the atomistic energetics of kink mechanisms in the leading and trailing partials with a full Peach-Koehler treatment of dislocation segment interactions and the stacking fault forces [8]. The results suggest a natural explanation of the low stress anomalies of dislocation mobility in semiconductors, including “the starting stress” and “the weak obstacles” effects. Work is underway to incorporate the atomistic kink mechanisms identified recently for BCC Mo and Ta, in a similar kMC model of screw dislocation motion. This is discussed later in the context of cross-slip.

Motion mechanisms of glissile and sessile jogs are being incorporated in the DD models and deserve to be explored atomistically. Atomistic simulations of the conservative jog motion are straightforward, at

approximately the same CPU cost as the 3D simulations of kink mechanisms. On the other hand, simulations of the sessile jogs dragging by screw dislocations will require more effort since vacancy or interstitial production is involved. The barriers for thermal activation of these non-conservative mechanisms are of prime importance and should be obtained by direct atomistic simulations. The results can be used to parameterize jog mobilities in the DD simulations and to replace the approximations currently used for the purpose.

2.3. CROSS-SLIP

In addition to the in-plane mobility just discussed, cross-slip is a mechanism by which dislocation motion becomes three-dimensional. As was recently demonstrated in a DD simulation, collective behavior of large dislocation ensembles is critically dependent on whether or not cross-slip is enabled [9]. For the DD models to become realistic, the cross-slip behavior of screw dislocations should be explored and quantified on an atomistic level. Recently, there has been considerable progress in this area. The most significant advance is due to Rasmussen et al, who explored 3D pathways for dislocation cross-slip in FCC Cu [10]. The results are consistent with the Friedel-Escaig (F-E) cross-slip mechanism in which a dissociated screw dislocation forms a finite length constriction and then re-dissociates into the cross-slip plane. The calculated activation barrier at zero stress is 3.0 eV. Despite the impressive computational machinery engaged in this simulation, the principal issue of the optimal cross-slip path remains unresolved for Cu and other FCC metals. This is because the outcome of the simulation (F-E path) was pre-determined by the symmetry of the initial state and by the choice of optimization method (conjugate gradients). Since it is rather likely that multiple paths for cross-slip exist, e.g. Fleischer mechanism [11] or jog-initiated cross-slip, they all deserve careful examination by direct atomistic simulation.

Cross-slip in BCC metals should be very different because, unlike FCC metals, screw dislocations are not confined to any particular plane by a planar dissociation: atomistic calculations suggest that screw dislocations either have a compact core or show a tendency to a non-planar, three-way extension. Cross-slip in BCC metals is nothing special, since screw dislocations do not have to constrict in the same sense as dislocations in FCC metals and should always have a choice of at least three {110} glide planes. Such behavior, when screw dislocations can translate in several planes, can be responsible for the well-known non-crystallographic “pencil” glide in BCC metals when dislocation motion follows rather accurately the Peach-Koehler force direction. At low to intermediate temperatures, both cross-slip and glide should take place by nucleation and propagation of kink pairs: the only difference between the glide

and cross-slip planes is the magnitude of shear stress resolved in each plane along the slip direction, i.e. the Schmid factor. The latter can be exactly the same for two close-packed planes of the <111> zone in which case the dislocation is equally likely to move in either plane. In such cases, kinks and jogs are indistinguishable and can be commonly referred to as "kogs". This situation, when two of the three available glide planes have nearly equal Schmid factors, can have interesting consequences for the motion of screw dislocations. Work is underway to incorporate the energetics of kog mechanisms in a kMC model for screw dislocation motion in BCC metals. Preliminary considerations indicate that dislocations can self-harden by a mechanism in which kogs produced in different planes collide and form pinning points which, in turn, can initiate jog dragging and formation of the debris of point defects and prismatic loops in the wake of dislocation motion.

3. Dislocation interactions

Here several issues of dislocation-dislocation interaction and dislocation-point defect interactions are discussed.

3.1. DISLOCATION COLLISIONS

The now famous cartoon from the Hirth-Lothe book illustrates very well the continuum and atomistic (core) stages in dislocation collisions [12]. The idea of that picture is expressed by a big question mark placed on top of the intersection point, implying that we know very little about the close range collisions when the cores of two intersecting dislocations begin to overlap. Although it remains unclear whether and how much the dislocation core contributes to the behavior of dislocations in collisions, recent atomistic simulations of dislocation reactions provide some interesting insights.

Bulatov et al analyzed results of a large scale MD simulation (by F. Abraham) of FCC solid containing a crack and observed that a Lomer-Cottrell (LC) reaction takes place between the dislocations emitted from the crack tip [13]. Junction formation proceeds by zipping, i.e. motion of the triple node points along the junction line and away from each other. Soon after the junction forms, another very interesting event takes place when a third dislocation approaches the first two, enters in a similar LC reaction with one of them and, subsequently, releases the other one of the two initial partners from the first junction reaction. The end result of such a "three-body" dislocation collision is that one of the two initial partners can continue gliding past the junction. This observation implies that even strong LC junctions are "penetrable" for

dislocation glide, through a junction replacement mechanism. In other words, even stable junctions can be destroyed by an incoming flux of primary or secondary dislocations. Subsequently, both elastic and core energy contributions to the energetics of the observed reactions were accurately calculated. When scaled to a typical length of colliding dislocations, say 0.5 microns in a cold-worked Cu, the elastic contribution was found to dominate the reaction energetics, consistent with the basic assumption of the Friedel-Saada line tension model.

Despite an initially repulsive arrangement, the intersection of two dissociated dislocations studied in [14] also produces a LC junction. For this to occur, two leading partial dislocations twist each other very significantly and join in an anti-parallel, locally attractive orientation. Continued forcing of one dislocation through the other results in junction unzipping and, eventually, dislocation cutting and jog formation. That such processes can occur even under constraints of unrealistically high forcing stress (from 400 MPa to 4 GPa) and short lengths of the intersecting lines, is supported by another 3D simulation of repulsive collisions (D. Rodney and R, Phillips, personal communication). It stands to notice that junction formation in both cases is consistent with the simple energy considerations (a modified Saada's rule taking into account the elastic anisotropy and the dislocation characters). The implication is that, when forced in contact, two initially repulsive dislocations can modify their approach trajectories to become locally attractive, which results in an energy reduction. This is achieved by bending either both (Zhou et al) or at least one (Rodney-Phillips) of the interacting partners and re-aligning them along the line of intersection of the two glide planes. It is nearly certain that a sufficiently refined DD simulation, a la Klaus Schwarz [15], would have predicted not only the outcome but also a significant part of the collision trajectory in all three cases of junction formation mentioned above. The only part that such a DD simulation can not handle properly is the specific details of dislocation core transformation during zipping and subsequent cutting. For this atomistic simulations are still required. The question is, should we really mire ourselves in such details? My answer to this is – it depends.

One situation in which core details should be rather unimportant in the dislocation reactions in soft FCC metals. For any given collision, what we must be primarily interested in is its outcome which can be one of the following: dislocations do not get in contact, dislocation approach and stay connected, and dislocation connect and pass through each other[1]. For dislocation lengths of practical interest, the energetics of dislocation collisions is determined nearly

[1] In cases when dislocation cutting occurs, energy of jog creation comes in the picture. It can be argued however that a fate of a given collision is pre-determined by forces other than cutting and the latter will not change the net outcome [16].

entirely by the elastic terms. And this elastic contribution is what matters, for as long as the outcome of a given reaction is governed by its energetics. The latter is likely to be the case in the collisions of the highly mobile glide dislocations in FCC metals. In some other situations, core details may have a significant effect on the junction behavior. As an example, even when the forces on its nodal points dictate junction unzipping, the response to these forces may not be immediate. In Si in particular, there should be a significant lattice resistance to motion of the nodal points along the junction line. At low temperature this resistance can be so high that an unstable junction will remain zipped for a very long time.

When the junction is stable, the core processes may still influence its behavior. One obvious example is a Lomer-Cottrell junction, which does not move in its {100} glide plane, due to a particular extension of its core into two intersecting {111} planes. It is because of this particular core configuration that the LC junction is expected to lock two parent dislocations, the implication being that the LC lock is absolutely sessile. Or is it? In 2D, motion of an extended LC junction dislocation is indeed nearly impossible. In 3D, however, glide in the {100} plane is possible, owing to the simple fact that all three dislocations involved in the LC reaction are parallel to a single {111} plane. This plane intersects the junction and also happens to be the common cross-slip plane of the parent dislocations. Therefore, if the triple node could move in that common plane, junction could move in its {100} plane, simultaneously pulling two glissile arms into their common cross-slip plane. Such a mechanism is not likely to operate if the node is extended: the energy required to form a constriction is very high in many FCC metals. On the other hand, one of the two triple nodes at the junction ends is often constricted for simple geometrical reasons – such a node is expected to glide relatively easily. Karnthaler [17] reported direct observations of {100} glide and of LC dislocations experiencing sessile-glissile transformations, suggesting that glide of LC locks is indeed possible. Since this behavior can have significant implications for the evolution of dense dislocation tangles in the cell walls, it is important to evaluate the atomistic pathways of nodal glide. So far we have calculated the energy of single kink formation on a LC dislocation in Al, at 0.17 eV, and in Cu, at 1.78 eV. These values indicate that the nodal glide mechanisms can be activated by temperature and stress and that their energetics are strongly dependent on the stacking fault energy.

3.2. DISLOCATION-POINT DEFECTS INTERACTION

Atomistic aspects of dislocation-point defect interactions are even less explored than dislocation-dislocation interactions. Considering the intrinsic defects,

vacancies and interstitials, full dynamics simulations are possible in certain situations, especially in view of the current advances in computer hardware and novel algorithms. An interesting example is dislocation motion in irradiated metals, where excess vacancies and interstitials can be present in the form of prismatic loops or stacking-fault tetrahedra. In this case, MD simulations can be effective if mobilities of dislocations and/or prismatic loops are high. In addition to possibly affecting the trajectories of moving dislocations through the elastic dislocation-loop interaction, collisions with prismatic loops can result in various dislocation-loop reactions. Outcomes of such reactions can be very interesting, including formation of super-jogs or enhanced cross-slip. In a way, this is similar to the mentioned above mechanism of debris production by screw dislocations in BCC, but in reverse. Another important target is the rate of dislocation climb, which can be sampled by direct MD simulations in certain cases. However, when climb rates are low, static methods may be more appropriate for obtaining the activation parameters of dislocation climb.

3.3. DISLOCATION-SOLUTE INTERACTIONS

Dislocation interactions with impurities and solute atoms are an area of great importance. In most practical situations, dislocation behavior is considerably different in the realistically “dirty” materials, as opposed to the ideal pure ones. Yield behavior in single crystalline Cu is one well-known example where dislocation mobility can vary by several orders of magnitude, depending on the specimen purity. Although continuum theory has provided considerable insight, our understanding of the physics of dislocation-solute interactions needs improvement and atomistic simulations can play an important role. In particular, non-linear effects of the dislocation core have not been studied in sufficient detail. Also, the core effects can influence dynamics of the Cottrell and Suzuki atmospheres.

The above-mentioned modes of dislocation-defect interactions can be incorporated, at least in principle, in the DD models in the form of re-normalized mobility laws. A more challenging problem is to account for the joint evolution of dislocation and alloy microstructures, especially in multi-component alloys and at large solute concentrations. Very little is known about possible synergistic mechanisms by which dislocations can be sources of partial local ordering or new phase formation and the emerging alloy microstructure can affect dislocation behavior. Methods of cluster-variation and semi-grand-canonical Monte Carlo appear to be good choices for exploring the thermodynamics of these processes. The major difficulty, in addition to the mentioned general problem of length and time scales, is the lack of reliable and computationally efficient models of interactions between the host lattice and the impurity atoms. In the hierarchy of models, from empirical potentials, to semi-

empirical TB and *ab initio* methods, one has to choose between reliability and efficiency. At present, the semi-empirical TB approaches often provide a reasonable compromise.

4. Summary

Current attempts to develop physically based descriptions of crystal plasticity raise the issue of linking atomistic and mesoscopic (continuum) descriptions of dislocation behavior. For new combined approaches to be predictive, rules for mesoscale simulations should be accurately matched to the atomistic mechanisms. This matching idea poses several general questions starting with the choice of degrees of freedom (DOFs) for setting up a mesoscale dislocation model. A "common sense" principle for selecting a particular mesoscopic representation is that, whatever DOFs are chosen, they must be identifiable both at the atomistic and the mesoscopic levels. In addition, the representation should retain maximum of the essential features of dislocation configurations at a minimal cost, to cut on the number of DOFs.

At present, several representations of dislocation lines have been advanced, including on- and off-lattice discretizations, linear and curved segments, various nodal representations, etc. Some of these map more naturally on the atomistic models while others offer computational advantages. Whatever scheme is used, matching between atomistic and mesoscopic descriptions involves two major aspects: (1) matching of the energies and forces acting on the chosen DOFs and (2) matching of the response of these DOFs to their conjugate forces. It appears that in most situations of practical interest, the forces on the mesoscopic DOFs (segments or nodes) come almost exclusively from the elastic terms. At the same time, the kinetics of dislocation response to these elastic forces resides with the dislocation core. Consequently, an accurate treatment of elastic interactions, including general anisotropy, is more important for obtaining the forces acting on dislocations. On the other hand, atomistic simulations can and should be used more to provide the rules for dislocation response to the elastic forces.

These and other issues can be addressed more effectively if continuum and atomistic modeling efforts are developed in parallel and the meso- and micro-modelers work alongside and interact continuously. The next 5-15 years are likely to produce new developments along these lines. From my own narrow viewpoint, I would like to see significant activities in the following areas of atomistic modeling:

(1) accurate evaluation of dislocation core structure and core energy, with increasing use of TB and DFT methods (semiconductors, BCC transition metals);
(2) MD simulations of dislocation motion, including kink and conservative jog mechanisms and cross-slip (using empirical interatomic potentials and, possibly, TB potentials);
(3) 3D modeling of dislocation junction behavior (static and dynamic, mostly with empirical potentials);
(4) 3D modeling of dislocation interaction with intrinsic point defects, including jog-dragging and debris loop production (static and dynamic, with empirical potentials and TB);
(5) thermodynamics of dislocation-solute interactions and stress-induced phase transformation in metallic alloys (TB and DFT).

In a longer run, I do not expect that the inevitable growth of CPU power will result in a straightforward increase of the system sizes attempting to simulate more and more complex dislocation arrangements. I think this kind of growth better be relegated to the mesoscale DD approaches. Rather, atomistic modeling should concentrate on the "unit" mechanisms of dislocation behavior but use more and more accurate (and CPU intensive) methods for the purpose. To see what may become possible let's assume that the Moore's law will remain accurate for the next 30 years, i.e. that the CPU speed will continue to increase by an order of magnitude roughly every 5 years. Let's take, as a very crude estimate, that the time step per atom is 1000 times costlier for an O(N) TB calculation than for a typical empirical potential, and that the same ratio will hold in the future between the O(N) DFT calculations and the O(N) TB methods. Then, TB calculations should be able to handle the problems of the same complexity as the present day simulations with empirical potentials, but with a time lag of 15 years, followed by the O(N) DFT methods, another 15 years behind.

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